

# Indexing Fe-phases in/on GaN using x-ray powder diffraction

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This document reports the x-ray powder diffraction main reflections (intensity threshold  $\geq 100$ ) for possible Fe-related phases forming during the metal-organic vapor phase epitaxy (MOVPE) growth of Fe in  $\text{NH}_3/\text{H}_2$  mixture on wurtzite-GaN/sapphire. The  $2\theta$  values are given for Cu  $K\alpha_1$  radiation (1.5406 Å) in the range 25-100 deg (ordered by increasing  $2\theta$ ). The GaN(000 $l$ ) and  $\text{Al}_2\text{O}_3$ (000 $l$ ) are also reported for reference. These data are obtained from the Inorganic Crystal Structures Database (ICSD, <http://icsd.fiz-karlsruhe.de/>). The access to ICSD has been provided by the European Synchrotron Radiation Facility (ESRF).

**Table 1:** Indexing Fe-phases in/on GaN using x-ray powder diffraction

Phase	Type	Spg.	HKL	$2\theta$	$d$ -sp.	M.	Int.	Ref.
$\epsilon$ -Fe <sub>2</sub> N		P312	101	29.52	3.0238	6	1000.0	[1]
$\epsilon$ -Fe <sub>3</sub> N		P312	101	29.54	3.0212	6	629.3	[2]
Fe <sub>24</sub> N <sub>10</sub>		P312	210	29.59	3.0163	6	444.3	[1]
Fe <sub>24</sub> N <sub>10</sub>		P312	120	29.59	3.0163	6	444.3	[1]
$\epsilon$ -Fe <sub>3</sub> N		P312	101	29.84	2.9915	6	641.1	[1]
Fe <sub>3</sub> O <sub>4</sub>	Al <sub>2</sub> MgO <sub>4</sub>	Fd-3mZ	220	30.09	2.9678	12	284.0	[3]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	210	31.93	2.8008	8	202.7	[4]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	104	33.12	2.7028	6	1000.0	[5]
Fe <sub>24</sub> N <sub>10</sub>		P312	300	33.66	2.6601	6	135.5	[1]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	112	34.00	2.6344	8	382.8	[4]
GaN	ZnS(2H)	P63mc	002	34.56	2.5931	2	360.5	[6]
Fe <sub>3</sub> O <sub>4</sub>	Al <sub>2</sub> MgO <sub>4</sub>	Fd-3mZ	311	35.44	2.5309	24	1000.0	[3]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	110	35.61	2.5190	6	732.7	[5]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	021	37.46	2.3988	4	150.9	[7]
$\epsilon$ -Fe <sub>3</sub> N		P312	110	37.53	2.3945	6	1000.0	[2]
$\epsilon$ -Fe <sub>2</sub> N		P-3m1	100	37.53	2.3946	6	275.5	[2]
$\epsilon$ -Fe <sub>2</sub> N		P312	110	37.55	2.3935	6	497.2	[1]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	110	37.56	2.3928	6	156.1	[8]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	100	37.64	2.3876	6	1000.0	[9]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	121	37.64	2.3878	8	267.9	[10]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	210	37.74	2.3818	4	244.5	[10]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	110	38.09	2.3604	6	184.5	[11]
$\epsilon$ -Fe <sub>3</sub> N		P312	110	38.13	2.3580	6	1000.0	[1]
Fe <sub>24</sub> N <sub>10</sub>		P312	220	39.07	2.3038	6	1000.0	[1]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	100	39.74	2.2664	6	255.2	[12]

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**Table 1:** Indexing Fe-phases in/on GaN using x-ray powder diffraction

Phase	Type	Spg.	HKL	2 $\theta$	d-sp.	M.	Int.	Ref.
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	202	39.78	2.2641	8	272.3	[4]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	002	39.79	2.2635	2	194.2	[10]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	110	40.07	2.2483	6	200.9	[13]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	201	40.62	2.2191	4	167.8	[10]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	220	40.71	2.2142	4	121.1	[4]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	002	40.72	2.2140	2	202.6	[9]
Fe <sub>24</sub> N <sub>10</sub>		P312	310	40.73	2.2134	6	170.0	[1]
Fe <sub>24</sub> N <sub>10</sub>		P312	130	40.73	2.2134	6	170.0	[1]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	200	40.77	2.2115	2	310.0	[7]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	002	40.81	2.2094	2	235.2	[11]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	002	40.82	2.2085	2	209.6	[8]
$\epsilon$ -Fe <sub>2</sub> N		P-3m1	002	40.89	2.2050	2	373.2	[2]
$\gamma'$ -GaFe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	111	41.14	2.1924	8	1000.0	[14]
(Ga <sub>0.5</sub> Fe <sub>0.5</sub> )Fe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	111	41.18	2.1905	8	1000.0	[14]
$\gamma'$ -Fe <sub>4</sub> N	CaTiO <sub>3</sub>	Pm-3m	111	41.22	2.1882	8	1000.0	[11]
Al <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	006	41.68	2.1650	2	1.5	[15]
$\epsilon$ -Fe	Mg	63/mmc	100	42.30	2.1348	6	256.8	[16]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	212	42.42	2.1292	16	1000.0	[4]
Fe <sub>3</sub> Ga	AuCu <sub>3</sub>	Pm-3m	111	42.53	2.1241	8	1000.0	[17]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	102	42.68	2.1166	4	500.2	[7]
$\alpha$ -Fe <sub>16</sub> N <sub>2</sub>		I4/mmm	202	42.70	2.1159	8	1000.0	[18]
$\gamma$ -Fe	Cu	Fm-3m	111	42.83	2.1099	8	1000.0	[19]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	121	42.85	2.1087	8	1000.0	[7]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	211	42.87	2.1078	8	576.0	[10]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	002	42.89	2.1070	2	267.4	[12]
$\gamma$ -FeN <sub>0.0950</sub>	$\gamma$ -FeN <sub>x</sub>	Fm-3m	111	42.93	2.1050	8	1000.0	[20]
$\epsilon$ -Fe <sub>2</sub> N		P-3m1	011	42.94	2.1044	6	1000.0	[2]
$\epsilon$ -Fe <sub>2</sub> N		P-3m1	101	42.94	2.1044	6	819.2	[2]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	111	42.95	2.1039	12	1000.0	[8]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	002	43.00	2.1018	2	247.7	[13]
Fe <sub>3</sub> O <sub>4</sub>	Al <sub>2</sub> MgO <sub>4</sub>	Fd-3mZ	400	43.07	2.0985	6	201.3	[3]
Fe <sub>24</sub> N <sub>10</sub>		P312	102	43.13	2.0958	6	209.7	[1]
$\alpha$ -FeN <sub>0.0950</sub>	$\alpha$ -FeN <sub>x</sub>	I4/mmm	101	43.15	2.0950	8	1000.0	[20]
$\gamma$ -Fe	Cu	Fm-3m	111	43.38	2.0842	8	1000.0	[21]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	111	43.43	2.0820	12	1000.0	[11]
$\alpha$ -Fe	W	Im-3m	110	43.63	2.0729	12	1000.0	[22]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	102	43.73	2.0684	4	565.9	[10]
Fe <sub>0.8</sub> Ga <sub>0.2</sub>	W	Im-3m	110	44.02	2.0556	12	1000.0	[23]
Fe <sub>3</sub> Ga	BiF <sub>3</sub>	Fm-3m	220	44.07	2.0531	12	1000.0	[24]
$\alpha$ -Fe	W	Im-3m	110	44.35	2.0407	12	1000.0	[25]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	220	44.56	2.0315	4	526.2	[10]
$\alpha$ -Fe	W	Im-3m	110	44.68	2.0267	12	1000.0	[19]
$\epsilon$ -Fe	Mg	P63/mmc	002	44.72	2.0250	2	285.4	[16]
$\alpha$ -Fe <sub>16</sub> N <sub>2</sub>		I4/mmm	220	44.78	2.0223	4	510.2	[18]
$\alpha$ -FeN <sub>0.0950</sub>	$\alpha$ -FeN <sub>x</sub>	I4/mmm	110	44.94	2.0153	4	473.3	[20]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	031	45.00	2.0127	4	1000.0	[10]

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**Table 1:** Indexing Fe-phases in/on GaN using x-ray powder diffraction

Phase	Type	Spgr.	hkl	2 $\theta$	d-sp.	M.	Int.	Ref.
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	101	45.40	1.9960	12	1000.0	[12]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	111	45.73	1.9825	12	1000.0	[13]
$\gamma$ -Fe	Cu	Fm-3m	111	45.78	1.9803	8	1000.0	[26]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	310	45.78	1.9805	8	561.4	[4]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	112	45.85	1.9774	8	487.1	[10]
Fe <sub>24</sub> N <sub>10</sub>		P312	112	46.17	1.9646	6	199.8	[1]
Fe <sub>24</sub> N <sub>10</sub>		P312	11 $\bar{2}$	46.17	1.9646	6	199.8	[1]
$\epsilon$ -Fe <sub>3</sub> N		P312	012	46.92	1.9348	6	168.8	[1]
$\gamma'$ -GaFe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	200	47.87	1.8987	6	557.0	[14]
(Ga <sub>0.5</sub> Fe <sub>0.5</sub> )Fe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	200	47.91	1.8971	6	558.2	[14]
$\gamma'$ -Fe <sub>4</sub> N	CaTiO <sub>3</sub>	Pm-3m	200	47.97	1.8950	6	569.3	[11]
$\epsilon$ -Fe	Mg	P63/mmc	101	48.18	1.8885	12	1000.0	[16]
$\epsilon$ -Fe <sub>2</sub> N		P312	021	48.47	1.8767	6	215.5	[1]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	131	48.60	1.8718	8	332.7	[10]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	221	49.11	1.8535	8	409.1	[10]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	024	49.42	1.8428	6	359.4	[5]
Fe <sub>3</sub> Ga	AuCu <sub>3</sub>	Pm-3m	200	49.51	1.8395	6	452.6	[17]
$\epsilon$ -Fe <sub>3</sub> N		P312	021	49.16	1.8519	6	145.1	[1]
$\gamma$ -Fe	Cu	Fm-3m	200	49.87	1.8272	6	448.5	[19]
$\gamma$ -FeN <sub>0.0950</sub>	$\gamma$ -FeN <sub>x</sub>	Fm-3m	200	49.99	1.8230	6	484.7	[20]
$\gamma$ -Fe	Cu	Fm-3m	200	50.52	1.8050	6	446.7	[21]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	122	51.82	1.7629	8	170.7	[10]
$\gamma$ -Fe	Cu	Fm-3m	200	53.38	1.7150	6	439.3	[26]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	116	54.00	1.6966	6	213.7	[5]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	11 $\bar{6}$	54.00	1.6966	6	213.7	[5]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	230	54.42	1.6847	4	116.1	[10]
$\gamma$ -Fe	Cu	Fm-3m	111	55.60	1.6517	8	1000.0	[27]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	004	56.08	1.6386	2	160.8	[4]
$\zeta$ -Fe <sub>2</sub> N		bcn	221	56.55	1.6260	8	176.6	[7]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	102	56.65	1.6235	12	764.3	[9]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	112	56.67	1.6229	12	189.7	[8]
Fe <sub>3</sub> O <sub>4</sub>	Al <sub>2</sub> MgO <sub>4</sub>	Fd-3mZ	511	56.96	1.6154	24	235.6	[3]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	112	57.05	1.6130	12	166.7	[11]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	301	57.98	1.5893	4	151.0	[10]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	102	59.89	1.5431	12	126.5	[12]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	112	60.22	1.5354	12	150.1	[13]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	12 $\bar{4}$	62.38	1.4873	6	141.2	[5]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	214	62.38	1.4873	6	141.2	[5]
Fe <sub>3</sub> O <sub>4</sub>	Al <sub>2</sub> MgO <sub>4</sub>	Fd-3mZ	440	62.54	1.4839	12	388.9	[3]
$\epsilon$ -Fe	Mg	P63/mmc	102	63.24	1.4692	12	123.7	[16]
$\alpha$ -Fe	W	Im-3m	200	63.41	1.4657	6	131.9	[22]
Fe <sub>2</sub> O <sub>3</sub>	Al <sub>2</sub> O <sub>3</sub>	R-3c:H	300	63.96	1.4543	6	270.2	[5]
Fe <sub>0.8</sub> Ga <sub>0.2</sub>	W	Im-3m	200	64.00	1.4535	6	133.1	[23]
Fe <sub>3</sub> Ga	BiF <sub>3</sub>	Fm-3m	400	64.09	1.4518	6	133.5	[24]
$\alpha$ -Fe	W	Im-3m	200	64.53	1.4430	6	130.3	[25]
$\alpha$ -Fe	W	Im-3m	200	65.03	1.4331	6	129.7	[19]

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**Table 1:** Indexing Fe-phases in/on GaN using x-ray powder diffraction

Phase	Type	Spg.	HKL	2 $\theta$	d-sp.	M.	Int.	Ref.
$\gamma$ -Fe	Cu	Fm-3m	200	65.16	1.4304	6	414.5	[27]
$\alpha$ -Fe <sub>16</sub> N <sub>2</sub>		I4/mmm	400	65.18	1.4300	4	130.2	[18]
$\alpha$ -FeN <sub>0.0950</sub>	$\alpha$ -FeN <sub>x</sub>	I4/mmm	200	65.44	1.4250	4	121.6	[20]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	023	67.34	1.3894	4	155.8	[7]
$\epsilon$ -Fe <sub>2</sub> N		P-3m1	110	67.72	1.3825	6	309.9	[2]
$\epsilon$ -Fe <sub>3</sub> N		P312	300	67.72	1.3825	6	287.6	[2]
$\epsilon$ -Fe <sub>2</sub> N		P312	300	67.75	1.3819	6	175.9	[1]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	300	67.78	1.3815	6	176.6	[8]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	110	67.94	1.3785	6	223.8	[9]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	412	67.96	1.3781	16	130.0	[4]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	300	68.83	1.3628	6	154.6	[11]
$\epsilon$ -Fe <sub>3</sub> N		P312	300	68.92	1.3614	6	282.8	[1]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	332	69.82	1.3459	8	110.1	[4]
$\gamma'$ -GaFe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	220	70.02	1.3426	12	277.6	[14]
(Ga <sub>0.5</sub> Fe <sub>0.5</sub> )Fe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	220	70.09	1.3414	12	275.8	[14]
$\gamma'$ -Fe <sub>4</sub> N	CaTiO <sub>3</sub>	Pm-3m	220	70.18	1.3400	12	295.8	[11]
Fe <sub>24</sub> N <sub>10</sub>		P312	600	70.78	1.3301	6	297.9	[1]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	123	70.81	1.3295	8	153.0	[10]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	110	72.13	1.3085	6	127.2	[12]
Fe <sub>3</sub> Ga	AuCu <sub>3</sub>	Pm-3m	220	72.63	1.3007	12	224.5	[17]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	300	72.80	1.2980	6	129.7	[13]
GaN	ZnS(2H)	P63mc	004	72.90	1.2965	2	25.9	[6]
$\gamma$ -Fe	Cu	Fm-3m	220	73.19	1.2920	12	217.1	[19]
$\gamma$ -FeN <sub>0.0950</sub>	$\gamma$ -FeN <sub>x</sub>	Fm-3m	220	73.39	1.2891	12	233.3	[20]
$\gamma$ -Fe	Cu	Fm-3m	220	74.24	1.2763	12	214.9	[21]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	314	75.20	1.2625	16	227.9	[4]
$\zeta$ -Fe <sub>2</sub> N		Pbcn	321	75.65	1.2561	8	128.5	[7]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	113	75.80	1.2540	12	157.7	[8]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	113	76.11	1.2496	12	151.7	[11]
$\epsilon$ -Fe <sub>3</sub> N		P312	113	76.50	1.2442	6	140.7	[1]
$\epsilon$ -Fe <sub>3</sub> N		P312	113	76.50	1.2442	6	140.7	[1]
$\alpha$ -Fe <sub>16</sub> N <sub>2</sub>		I4/mmm	224	76.71	1.2414	8	108.2	[18]
$\epsilon$ -Fe	Mg	P63/mmc	110	77.36	1.2325	6	116.9	[16]
$\alpha$ -FeN <sub>0.0950</sub>	$\alpha$ -FeN <sub>x</sub>	I4/mmm	112	77.84	1.2261	8	127.7	[20]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	401	77.89	1.2255	4	145.1	[10]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	133	78.58	1.2165	8	191.3	[10]
$\gamma$ -Fe	Cu	Fm-3m	220	78.87	1.2127	12	207.0	[26]
$\alpha$ -Fe	W	Im-3m	211	80.13	1.1968	24	222.6	[22]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	103	80.35	1.1939	12	130.2	[12]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	113	80.74	1.1892	12	126.8	[13]
Fe <sub>3</sub> Ga	BiF <sub>3</sub>	Fm-3m	422	81.06	1.1853	24	228.2	[24]
$\alpha$ -Fe <sub>16</sub> N <sub>2</sub>		I4/mmm	422	81.10	1.1848	16	198.0	[18]
$\alpha$ -Fe	W	Im-3m	211	81.65	1.1782	24	220.5	[25]
$\alpha$ -FeN <sub>0.0950</sub>	$\alpha$ -FeN <sub>x</sub>	I4/mmm	211	81.65	1.1783	16	203.0	[20]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	302	82.25	1.1712	12	140.6	[8]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	112	82.33	1.1702	12	110.8	[9]

Continued on next page

**Table 1:** Indexing Fe-phases in/on GaN using x-ray powder diffraction

Phase	Type	Spgr.	HKL	2 $\theta$	d-sp.	M.	Int.	Ref.
$\alpha$ -Fe	W	Im-3m	211	82.34	1.1701	24	219.7	[19]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	332	83.02	1.1622	8	200.4	[10]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	302	83.23	1.1599	12	140.6	[11]
$\epsilon$ -Fe <sub>3</sub> N <sub>1.39</sub>	Mn <sub>2</sub> N <sub>1-x</sub>	P6322	221	83.68	1.1548	12	118.8	[8]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	251	83.91	1.1522	8	110.2	[10]
$\gamma'$ -GaFe <sub>3</sub> N	CaTiO <sub>3</sub>	Pm-3m	311	84.56	1.1450	24	244.3	[14]
$\gamma'$ -Fe <sub>4</sub> N	CaTiO <sub>3</sub>	Pm-3m	311	84.76	1.1427	24	266.4	[11]
$\epsilon$ -Fe	Mg	P63/mmc	103	84.92	1.1410	12	128.1	[16]
$\epsilon$ -Fe <sub>3</sub> N	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	221	84.99	1.1403	12	108.2	[11]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	303	86.16	1.1278	4	123.2	[10]
Fe <sub>0.7</sub> Ga <sub>0.3</sub>	Mg	P63/mmc	112	87.73	1.1116	12	131.6	[12]
Fe <sub>3</sub> Ga	AuCu <sub>3</sub>	Pm-3m	311	87.97	1.1093	24	236.0	[17]
Fe <sub>3</sub> C	Fe <sub>3</sub> C	Pnma	430	88.13	1.1076	4	128.8	[10]
$\epsilon$ -Fe <sub>3</sub> C	Fe <sub>3</sub> N <sub>1+x</sub>	P6322	302	88.45	1.1044	12	110.6	[13]
$\gamma$ -Fe	Cu	Fm-3m	311	88.71	1.1018	24	227.5	[19]
$\gamma$ -FeN <sub>0.0950</sub>	$\gamma$ -FeN <sub>x</sub>	Fm-3m	311	88.97	1.0993	24	229.3	[20]
FeGa <sub>3</sub>	FeGa <sub>3</sub>	P42/mnm	522	89.30	1.0960	16	149.5	[4]
$\gamma$ -Fe	Cu	Fm-3m	311	90.09	1.0885	24	227.1	[21]
$\epsilon$ -Fe	Mg	P63/mmc	112	94.05	1.0528	12	128.1	[16]
$\epsilon$ -Fe <sub>2.3</sub> N	NiAs	P63/mmc	202	94.29	1.0508	12	127.9	[9]
$\gamma$ -Fe	Cu	Fm-3m	311	96.29	1.0342	24	230.0	[26]
$\gamma$ -Fe	Cu	Fm-3m	220	99.20	1.0114	12	213.9	[27]

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